PETSC and TAO hands-on Notes

High Performance Software Tools to Fast-Track The Development of Scalable and Sustainable Applications

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Outline

- Quick reminder of the supercomputer use at NERSC
- PETSc
- TAO

Accessing carver and today's ACTS tools

Log-in to carver:

- `ssh -X train[]@carver.nersc.gov`

Upload the PETSc

- `Module load petsc/3.1_g` *(for -g version)*
- `Module load petsc/3.1_O` *(for -O3 version)*
- `Module load petsc/3.1_g_c++` *(for c++ bindings)*
- `Module load petsc/3.1_g_complex` *(for complex)*

(you can also use 3.1_O_c++ or 3.1_O_complex)

Using the module command you will automatically set the environment variables: PETSC_DIR and PETSC_ARCH

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Upload the TAO

- `Module load tao/1.10.1_g` *(for -g version)*
- `Module load tao/1.10.1_O` *(for -O3 version)*

Using the module command you will automatically set the environment variables: TAO_DIR, PETSC_DIR and PETSC_ARCH

Accessing carver and today's ACTS tools

Upload the superlu and superlu_dist

- `Module load superlu_dist/2.3_g` *(for -g version)*
- `Module load superlu_dist/2.3_O` *(for -O3 version)*

Using the module command you will automatically set the environment variables: SUPERLU_DIST_EXAMPLE, SUPERLU_DIST and SUPERLU_DIST_SRC

Running on Magellan

You need to use a script to launch your executables:

```
#!/bin/tcsh
#
#PBS -l walltime=00:02:00
#PBS -l nodes=<select number of nodes (1 node = 8
cores)>
#PBS -q mag_acts
#PBS -N <give a name to your job>

cd $PBS_O_WORKDIR
module load mkl
mpirun -np <number_procs> ./<your_executable_name>
```